# APPENDIX C

# CHARACTERIZING VARIABILITY AND UNCERTAINTY IN THE CONCENTRATION TERM

## C.0 THE CONCENTRATION TERM AND THE EXPOSURE UNIT

Incomplete knowledge of the concentration of one or more chemicals in various exposure media is often the major source of uncertainty in Superfund risk assessments. In any risk assessment, the derivation of the concentration term will reflect assumptions about: (1) properties of the contaminant, (2) the spatial and temporal variability in contamination, (3) the behavior of the receptor, and (4) the time scale of the toxicity of the chemical(s). This appendix expands upon concepts introduced in Chapter 5. This appendix does not provide detailed equations for performing calculations, but instead refers the reader to other Environmental Protection Agency (EPA) guidance documents in which both the recommended approaches and calculations are provided.

The concentration term is linked to the concept of an exposure unit (EU). For Superfund risk assessments, an EU is the geographical area in which a receptor is randomly exposed to a contaminated medium for a relevant exposure duration. Environmental sampling provides information about the contamination within and around an EU. Multiple EUs may be defined at a site based on the choice of a receptor, the exposure medium, and the nature of contact with the medium. For example, residential exposures to children may involve exposures via soil and dust ingestion both at the primary residence and recreational areas at a day care facility. Site-specific information regarding the activities of receptors should guide assumptions about the receptor's contact with exposure media.

> ☞ *Defining the EU is critical to the success of the remedial strategy, as it affects the calculation of the concentration to which receptors are exposed.*

## C.1.0 VARIABILITY IN PRA

In general, variability and uncertainty should be kept separate to the extent possible in any probabilistic risk assessment (PRA). For example, assume a one-dimensional Monte Carlo Analysis (1-D MCA) was developed to characterize variability in risk, but it combined a distribution for uncertainty in mean concentration with distributions for variability in exposure variables. The result would yield a single distribution for risk, however, each risk estimate would reflect both uncertainty and variability and distinguishing between the two would not be possible. Therefore, EPA's *Guiding Principles for Monte Carlo analysis* recommends against mixing distributions of variability and uncertainty in a 1-D MCA (U.S. EPA, 1997b) to avoid such ambiguities.

A fundamental concept in Monte Carlo analysis is that there is variability in exposure between receptors (inter-individual variability) as well as day-to-day variability for each individual (intra-individual variability). In most Tier 2 analyses (see Chapter 2), the goal of a 1-D MCA is to characterize inter-individual variability in exposure and risk. Typically, probability distributions for exposure represent variability (PDFv's) between individuals in the average value over the entire exposure duration. In this case, the exposure point concentration (EPC) should represent the average exposure concentration

over the entire exposure duration. Because an EPC is calculated from a sample, there is uncertainty that the sample mean equals the true mean concentration within the EU; therefore, to account for associated uncertainty, the 95% upper confidence limit for the mean (95% UCL) is generally used for Superfund risk assessments (U.S. EPA, 1992).

In a 1-D MCA, a point estimate for the EPC is combined with PDFv's for other variables to yield a probability distribution for risk. An alternative approach is to simulate long-term average exposures as a series of consecutive short-term exposure events. This approach is referred to as MicroExposure Event (MEE) Monte Carlo modeling, and is discussed in detail in Appendix D. In MEE modeling, the goal is to develop PDFv's for exposure variables that capture the event-to-event variability in exposures at the individual level. The concept of an averaging time still applies, but generally to a shorter time frame. For example, seasonal variability in exposure frequency might be expected among outdoor occupational workers so that different PDFv's are representative of inter-individual for each season. In this case, the EPC continues to represent an average concentration within the EU, but it would be linked to season-specific activity patterns. It may be important to develop two different weighted averages to reflect season-specific activity patterns and locations that are more frequently contacted in the summer compared with the winter, for example. As the time frame for the exposure scenario is shortened from the entire exposure duration, to a season, to a day, to an individual event, the concentration term should be reevaluated to assess the relevance of the assumption that concentrations contacted by the receptor are represented by the mean of the measured sample.

The following discussion introduces concepts of temporal and spatial variability as they apply to the estimate of the EPC for different exposure media and exposure scenarios. While the general rule of thumb applies to all Monte Carlo models—use a measure of the average concentration within the EU over the time frame of exposure—it is important to apply the site sampling data in a way that is consistent with the exposure scenario.

### C.1.1 TEMPORAL VARIABILITY

Temporal variability in chemical concentrations may be an important consideration when developing a preliminary remediation goal (PRG) for any exposure medium (refer to Chapter 5 for a comprehensive discussion of using PRA to evaluate PRGs). For example, wind erosion may change chemical concentrations in surface soil over time; leaching may change concentrations in both subsurface soil and groundwater; and bioaccumulation may result in increasing concentrations in predatory fish with time. If possible, such factors should be considered early in the risk assessment process and included in the conceptual site model.

Development of the EPC normally will depend on the averaging time relevant to the exposure scenario and health endpoint of concern. In the shorter term, it may be unlikely that receptors are exposed throughout the entire EU due to temporal (and spatial) variability in the contaminant and inter-individual variability in activity patterns. Therefore, inter-individual variability in the EPC might be expected, and a distribution of EPCs may be developed to represent differences in exposure among the population. Variability in short-term exposure may be an important factor for assessing variability in acute toxicity. However, over time, short-term variability in the EPC will tend to smooth out and approach a long-term average concentration. A single estimate of the long-term average EPC may be reasonable to use in assessing risks to the receptor population. This is true regardless of the underlying distribution of the environmental sampling data (e.g., lognormal, normal, beta, etc.).

While most chemicals regulated by the Superfund program are based on concerns for chronic toxicity (e.g., lifetime cancer risk from exposure to a carcinogen for ten or more years), for some chemicals, toxic effects occur with shorter exposure durations (e.g., nitrate in drinking water and methemoglobinemia in infants). Differences between acute and chronic health endpoints are important to consider for ecological receptors such as transient migratory species. Superfund guidance distinguishes between acute and chronic exposure to provide risk assessors the option of evaluating risk under different time frames. The EPC should be estimated within an EU during a period of time that has toxicological relevance for the exposed population.

☞ *The time scale of the concentration term should match the time scale of the toxicity criterion and exposure duration.*

### C.1.2 SPATIAL VARIABILITY

Spatial variability in chemical concentrations is also an important property to consider when developing a PRG. Spatial variability arises from many factors, including the mechanism of contamination, physical and chemical dilution and transformation processes, and physical characteristics of the site (Cullen and Frey, 1999). Similarly, receptors may exhibit spatial variability in their contact with an exposure medium. In general, receptors are assumed to have equal access to all areas within an EU so that the concept of a long-term average concentration is applicable.

Often, the EPC is estimated without regard to the spatial patterns in contamination. The sampling design yields a measure of the variability in concentrations that is assumed to be representative of the receptor's contact with the exposure medium. However, even when the sampling design is representative (e.g., both are simple random samples within the EU), the concentrations may exhibit clear spatial patterns that could be used to reduce uncertainty in the EPC. Geostatistics (see Section C.5.2 and Appendix D) offers a wide range of techniques for incorporating spatial information into estimates of the EPC. These techniques are particularly useful when there is uncertainty in the representativeness of site sampling, due to a difference in scale between site sampling and the size of the EU, or the use of targeted sampling designs that oversample areas within an EU believed to contain the highest levels of contamination.

In point estimate risk assessments (Tier 1 of the PRA), the EPC is most often characterized by a point estimate of the mean concentration, typically given by the 95% UCL for the mean to account for uncertainty in the site characterization (U.S. EPA, 1992). Variability in concentrations is an important consideration for determining appropriate statistical methods used to estimate the 95% UCL. In addition, for some Monte Carlo models, a PDFv may be developed to determine the EPC for the exposure model. A PDFv for the EPC may be warranted in short-term exposure scenarios, particularly when the sampling density is relatively sparse in relation to the size of the EU (i.e., poor site characterization). For example, a risk assessment may include a future use residential scenario (e.g., currently the site is undeveloped) in which the EPC that is relevant to a potentially exposed population of children is the average concentration within a 0.5 acre lot. If the soil sampling yields 100 measurements, but a small subset of the samples (e.g., less than three) are available for any 0.5 acre area, the most appropriate measure of the average concentration for a hypothetical residence may be the maximum detected concentration or a single value from the PDFv in concentration among hypothetical receptors. In general, for any of the EU's that define a randomly located residence, the poor site characterization would be a source of uncertainty in both a point estimate and probabilistic risk assessment.

At the vast majority of sites, concentration data is the easiest data to obtain of all the exposure variables. In cases of poor site characterization, risk managers may opt to perform a point estimate risk assessment only using the maximum detected concentration and highly protective exposure assumptions. In the scenario described above for 0.5 acre residential lots, it is possible that a residence would be located in an area in which the average concentration is represented by the maximum detected concentration in the sample. Should the risk manager opt for a Tier 1 point estimate risk assessment, the use of the maximum detected concentration of a chemical on the site should ensure the performance of a health-protective risk assessment within a smaller EU.

Consideration of variability is also warranted in short-term scenarios for ecological risk assessment (ERA) when the EU is much smaller than the site (see Section C.3.1.1). For example, the home range of the receptor populations may be relatively small in comparison to the spatial distribution of sampling locations (e.g., benthic invertebrates living in the sediment at the bottom of a river or soil invertebrates in a terrestrial habitat). In these cases, the receptor would be exposed to an area smaller than the sampling grid or measure of areal sampling density. A value from the PDFv that characterizes variability in the concentrations across a relatively large spatial scale may be used to define the EPC for a receptor population at a smaller scale. Again, risk assessors should take care in designing a 1-D Monte Carlo model when using a PDFv for the concentration term. It is unadvisable to mix a PDFv for the concentration term with PDFv's for other exposure scenarios when estimating risks within one EU. Use of the PDFv in this manner would incorrectly suggest that the mean concentration varied for each individual within the same EU according to the variability in concentration measured across a much larger area. A preferred approach is to use a PDFv to obtain a point estimate that represents the EPC, and then combine this point estimate with PDFv's for other variables in the Monte Carlo simulation to estimate risks in the small EU. If there are many EU's at a site, or if the boundaries of EUs are undefined, more advanced modeling approaches can be developed to efficiently run multiple scenarios. Methods for characterizing exposure point concentrations for ecological receptors are further discussed in Sections C.2 and C.3.

### C.1.3 Example of Temporal and Spatial Variability

Exposure scenarios often require consideration of both temporal and spatial variability. The MEE might be used to assess temporal variability by simulating long-term intake as the sum of individual exposure events. The time step for MEE is an important consideration and will depend on the rate of change of the most rapidly changing exposure variable. In addition, there should be a correspondence between the time periods over which data were obtained and the time step used in the MEE model. For example, when a MEE is used for the risk assessment, the concentration term selected at each time period should match the "average" concentration within the EU appropriate for that particular time period. Assume that the receptor is a residential child, and the time period is a single day, and the child may contact only 1,000 square feet within the 0.5 acre (20,000 square feet) residential EU. The specific 1,000 square foot area may change with each day as the child chooses different areas in the yard to frequent. Hence, the variability in the sample may be a more appropriate measure of the concentration contacted by residential child receptor on a day-to-day basis than the long-term average within the 0.5 acre EU. Over the long-term, this receptor will be exposed to the entire EU and hence the average contaminant concentration within the 0.5 acre EU. Note that the day-to-day variability in concentration undergoes the familiar phenomenon of "regression to the mean" when considered over the long-term.

## C.1.4 Spatial and Temporal Variability for Different Exposure Media

### C.1.4.1 Variability of Concentrations in Soil

Surface soil is subject to erosion by wind and surface water runoff. Over time, concentrations in surface soil may change, but generally at a slow rate relative to other media. The spatial variability of chemical contamination is most often due to the mechanism by which the contamination occurred. For example, particulate stack emissions will tend to fall in an even pattern downwind of the stack whereas over-application of pesticides and chemical spills can result in a patchy pattern of contamination.

Subsurface soil is not subject to wind erosion, so concentrations change mostly due to degradation processes or leaching of the contaminant to groundwater. At most Superfund sites, concentrations of chemicals in subsurface soil will remain relatively constant.

### C.1.4.2 Variability of Concentrations in Groundwater

Exposure to groundwater contamination mostly occurs at a fixed point in space (e.g., the wellhead). Groundwater is subject to a variety of influences that can alter chemical concentrations within this medium such as aerobic and anaerobic biodegredation, volatization, and absorption. Due to these influences, monitored natural attenuation is an appropriate remedy under certain site conditions. If a risk assessor wishes to use a measure of the long-term average of a concentration in groundwater, a hydrogeologist should be consulted.

### C.1.4.3 Variability of Concentrations in Surface Water

Concentrations in surface water can be very dynamic. Streams are constantly flowing and the effects of mixing, dilution and evaporation can change the chemical concentrations in surface water over relative short time periods. Any sampling of surface water is truly a "snapshot" in time. The sampling methods used to characterize spatial and temporal variability of concentrations in surface water will have a direct effect on the uncertainty in estimates of the average concentration over both short and long time frames.

### C.1.4.4 Variability of Concentrations in Sediment

In some situations, sediment may be considered a relatively stable medium, similar to soil. Alternatively, sediment may be physically moved by currents, tides, the movement of ships and other events. Trend analysis may be used to establish the long-term average sediment transport at a site. This information could provide the basis for choosing a representative "average" concentration in the sediment available to ecological receptors (Piest and Miller, 1975; Van Sickel and Beschta, 1983; Walling, 1983; Meade et al., 1990).

### C.1.4.5 Variability of Concentrations in Fish

Concentrations in fish may vary due to a change in the availability of food and environmental conditions. Factors that may be used to model population dynamics may include intensity of angler harvest, death/attrition of the population, and the introduction of a predator species or a more adaptive species. In risk assessments that include a fish ingestion exposure pathway, the activities of the angler may be a more important factor in determining the EPC than the changes in concentrations in fish over

time. For example, an avid recreational angler may harvest fish from different locations within a lake and consume fish of different sizes and species. In this way, with the consumption of contaminated fish, both the contaminated medium and the exposure point change throughout the exposure duration.

Unless, samples of fish are collected over time, knowledge of these factors will generally be unknown. Concentrations of bioaccumulative chemicals in territorial fish (e.g., largemouth bass) obtained in different locations will generally reflect the concentrations in the sediment in the individual's home territory. Concentrations of bioaccumulative chemicals in migratory fish will be more difficult to predict as the fish will contact areas with varying sediment and surface water concentrations.

### C.1.4.6 Examples of Temporal and Spatial Variability in the Concentration Term for Selected Exposure Media

Whatever medium is considered in the development of EPCs, the risk assessor should be aware that the EPC embodies aspects of both the spatial distribution of contamination, the movement of the receptor, and possibly the contaminated medium within the EU. Table C-1 presents examples of sources of temporal and spatial variability in the concentration term based on both the contamination in selected exposure media and the receptor.

**Table C-1**. Examples of temporal and spatial variability in selected media for the concentration term in common exposure scenarios.

| Factor | | Soil | Groundwater | Fish |
|---|---|---|---|---|
| Temporal Variability | Contaminant | • none, if contaminant source is inactive<br>• aerial deposition from ongoing source emissions affected by wind patterns<br>• degradation over time<br>• volatilization<br>• migration to groundwater<br>• radioactive growth and decay | • seasonal fluctuation in groundwater table<br>• migration of contaminant plume<br>• natural attenuation | • seasonal changes in species availability<br>• bioconcentration<br>• long-term changes in population dynamics<br>• fish tissue concentrations linked to temporal variability in water and sediment concentrations<br>• physical and chemical processes |
| | Receptor | • changes in activity patterns and behaviors over time (e.g., with age) | • none, fixed location at specific wellhead<br>• changes in well location over time | • dietary preferences for fish species<br>• cooking practices |
| Spatial Variability | Contaminant | • heterogeneity in concentrations over a small area and with depth, including presence of hotspots<br>• heterogeneity in soil properties that influence bioavailability | • migration of contaminant plume, based on hydrogeology and source emissions (e.g., bulk flow or continuous source) | • migration of fish<br>• changes in fish population structure |
| | Receptor | • daily activity patterns involve contact with different areas of the EU | • none, fixed location at specific wellhead<br>• changes in well location over time | • change in recreational habits, and areas fished |

## C.2.0 NONRANDOM EXPOSURES

As discussed in Section C.1.2, in the long-term it is generally assumed receptors exhibit random movement, such that there is an equal probability of contacting any area within the entire EU. Therefore, the long-term exposure concentration will most likely be the arithmetic mean of the concentration within the EU. However, in many situations, the assumption of random exposures in space may clearly be an oversimplification. People's behavior and preferences will cause them to access specific areas within an EU with greater frequency than others. The same is true in terms of ecological receptors with specific habitat preferences.

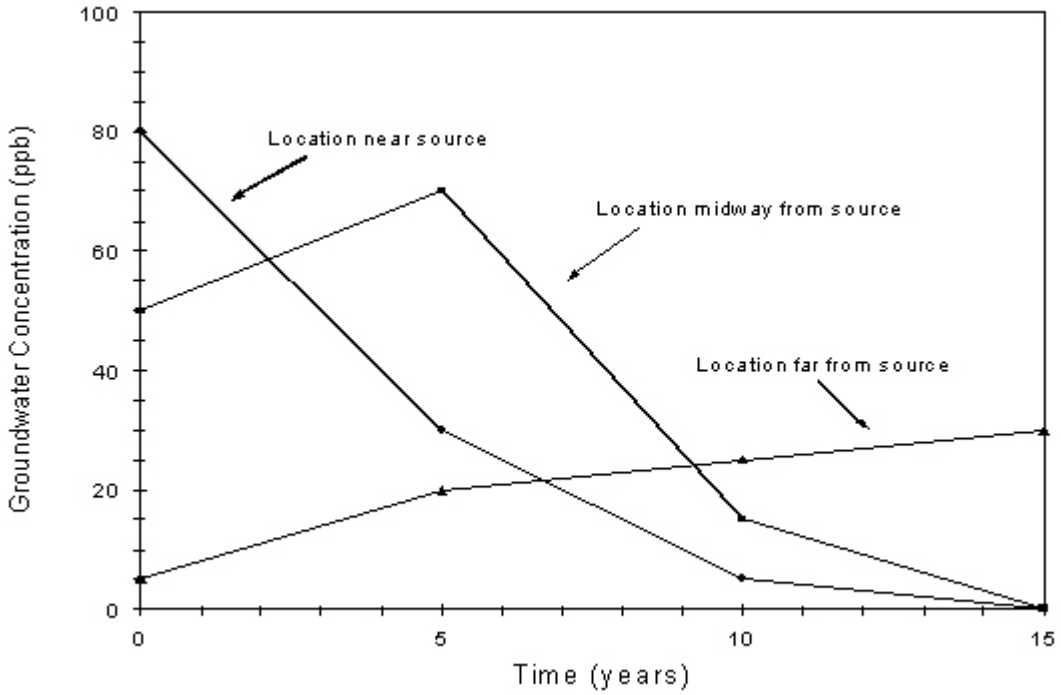


**Figure C-1.** Spatial and temporal variability in contaminant concentrations in groundwater.

For example, groundwater concentrations may show a large variation when sampled from wells in different locations (Figure C-1). Typically, residential receptors do not sample randomly from different wells, but draw chronically from individual wells. In such a case, the EU is a single wellhead. Fluctuations in the groundwater plume will depend on the hydrogeology of the site as well as the seasonal fluctuations in the water table. In this hypothetical example, concentrations are declining over time at distances nearest to the source, and concentrations are increasing as the plume moves farther from the source.

Incomplete information regarding the behavior patterns of people and environmental systems can be a large source of uncertainty in a risk assessment. Because of this, methods are being developed to model spatial relationships (between the contaminant and receptor) and nonrandom exposures. Recently, a quantitative technique to model nonrandom exposure has been proposed for ERA (Hope, 2000, 2001). Briefly, this technique divides the EU into smaller subunits and uses information about the attractiveness

of each subunit to assign a probability of the receptor occupying a given subunit for a period of time. Receptor movements are modeled stochastically and a time-weighted average of all the subunits provides a measure of the EPC. In some ecological risk assessments, telemetry data can be used to better characterize the areas of contamination that overlap with habitats of selected species. Hoff (1998) demonstrates an approach for American badgers (*Taxidea taxus*) in which telemetry data and geostatistical modeling provide an improved relationship between contaminant concentrations, tissue residues, and effects.

## C.3.0 SOURCES OF UNCERTAINTY IN THE CONCENTRATION TERM

There are numerous potential sources of uncertainty in the estimate of the true mean concentration within an EU. As discussed in Chapter 5 (Section 5.1.1), sources of uncertainty can be grouped into four broad categories: sample data, location of the EU, behavior of the receptor, and from miscellaneous sources (e.g., physical and chemical processes). Development of an uncertainty distribution for the average concentration requires knowledge of the variability in chemical concentrations within the EU (unless distribution-free approaches are used), the toxicity of the chemicals, and the receptor's behavior. These distributions should be developed by risk assessors with the concept of the EU in mind. Differences in scale (e.g., small home range of an ecological receptor population relative to the site sampling design) can be a major source of uncertainty in ecological risk assessments. Methods for addressing such uncertainties in the concentration term are presented below. By incorporating these methods into the quantitative uncertainty analysis, risk managers may more effectively evaluate the importance of data-gaps and design subsequent rounds of site sampling to reduce the uncertainty in the EPC.

## C.3.1 QUANTIFICATION OF UNCERTAINTY BASED ON THE SIZE OF THE EXPOSURE UNIT

Site characterization sometimes occurs before an EU has been defined. Therefore, an EU may be smaller than an entire site, equal to the site itself, or larger than the site. These three conditions lead to different conclusions and methods about the determination of the EPC. The most complex situation is when the EU is smaller than the site and the site can contain multiple EUs. For future scenarios in which the land use differs from the current land use, the difficulty in predicting the exact size and location of EUs necessitates accounting for the uncertainty in the EU.

Composite sampling is often used to maximize site information. However, it is important to note that the use of composite sampling influences the concentration term. If composite sampling is used exclusively at a site, the actual maximum concentration present or the best estimate of this maximum concentration will not be available. Depending on the time scale of the toxic effect or whether acute toxicity should be considered, this lack of knowledge of the maximum concentration present may be a large data gap. Risk assessors are urged to consider composite sampling and its ramifications for the concentration term.

### C.3.1.1 WHEN THE EXPOSURE UNIT IS SMALLER THAN THE SITE

The size of the EU will be different depending on the length of exposure. A receptor can access a greater area if given more time. In almost all cases, the size of the EU for short-term exposure will be smaller than the EU for long-term exposure. Therefore, in addition to the uncertainty associated with sampling and analysis (which can be quantified with existing methods for calculating confidence intervals), there is uncertainty about the location of the EU within the site.

If contamination is evenly spread across the site, the location of the EU may not have any bearing on the EPC. In such a case, uncertainty may depend on the sample size or density of measurements within the EU relative to the entire site. In point estimate risk assessments, the concentrations of chemicals at the sampling location that poses the greatest risk may be considered as estimates of the EPC for this small EU. Using this "riskiest" sampling location as an estimate of the mean within an EU of unknown location accounts for both the uncertainty associated with limited sampling within a single EU and the uncertainty of the location within the site of the EU.

To express the uncertainty in location of the EU as a distribution, methods have been developed to place an EU of a given size randomly about a site (Burmaster and Thompson, 1997). A concentration term is developed for each of a large number of randomly located EUs. The distribution of these concentration terms will express the uncertainty in the location of the EU.

Risk assessors are cautioned to consider whether the statistical method used to estimate the EPC in an EU accounts for all sources of uncertainty in the concentration term. If only a few samples are used to characterize the average concentration within an EU, then the uncertainty in the EPC is large and should be presented in the risk characterization. These conditions may warrant additional sampling or the use of analytical methods that account for spatial variability within the entire site.

At some sites, geostatistical methods, pattern recognition, and geographical information systems (GIS) methods may provide additional insight and will aid in the development of the concentration term (see Section C.5.2). Although Table 3-1 shows several statistical methods for estimating both point estimates and distributions that encode uncertainty in the concentration term, a risk assessor's understanding of these uncertainties should be conceptual as opposed to purely statistical.

#### C.3.1.2 When the Exposure Unit is the Same Size as the Site

In this case, the entire environmental data set within the site boundaries can be used for the determination of the concentration term. Assuming the EU occupies the entire site, then the source of uncertainty associated with knowing the average concentration within the EU is the sampling and analytical uncertainty.

#### C.3.1.3 When the Exposure Unit is Larger than the Site

In this case, the EU extends beyond the site boundaries. Therefore, the entire environmental data set within the site boundaries can be used for determination of the concentration term. However, an additional term in the exposure assessment may be needed to account for the fraction of the exposures that are expected to occur off site. Essentially, the contribution of the chemical concentrations measured on and off site are weighted by the fraction ingested or contacted in each area. Similarly, the term "area use factor" is used in ecological risk assessments to refer to the percentage of time or area an animal inhabits a contaminated area. An exposure scenario in which the EU is defined by the multiple locations that may be visited would be a common extension of this concept. One reasonable assumption regarding off site exposures is that the concentrations would be equal to the "background" concentrations. If this assumption is made, a site risk assessor should be consulted to determine appropriate methods for incorporating background concentrations into the risk assessment. Alternatively, additional sampling at off site locations would be needed to estimate the concentrations.

## C.4.0 SUMMARY OF RECOMMENDATIONS FOR THE CONCENTRATION TERM

Table C-2 presents general guidelines for establishing a concentration term in various media based on exposure time and the size of the EU. These general guidelines along with site-specific exposure conditions are the driving factors in risk assessment decision making for establishing the concentration term.

**Table C-2.** Summary of factors that may be considered in developing an EPC.

| Medium | Exposure Time | Random | Non-Random | Size of EU relative to the site/sampling density | Recommendation (Human Health and Ecological) |
|---|---|---|---|---|---|
| Soil | Short-term | | X | small | HH - consider variability in concentration relative to the time scale of toxicity.<br>ECO - time weighted average of smaller subunits. |
| Soil | Long-term | X | | variable | HH, ECO - consider uncertainty in the average concentration within an EU. |
| Fish | Short-term | | X | variable | HH, ECO - consider variability in sample concentrations relative to the exposure time. |
| Fish | Long-term | X | | variable | HH - consider uncertainty in the average concentration in consumed portion of fish.<br>ECO - consider uncertainty in average concentration of whole fish. |
| Ground-water | Short-term | | X | small - single well head | HH - consider either the highest detected concentration or uncertainty around the concentration at the center of the plume as a measure of a single well and relate to the time scale of the toxic effect.<br>ECO - not applicable |
| Ground-water | Long-term | | X | small - single well head | HH - consider variability among the higher concentration samples as a protective EPC. Alternatively, hydrogeologic modeling may be used to obtain a long-term average concentration in the most contaminated area.<br>ECO - not applicable |

## C.5.0 METHODS FOR ESTIMATING UNCERTAINTY IN THE MEAN CONCENTRATION

Confidence intervals (CIs) and UCLs are computed to characterize uncertainty in a parameter estimate. CIs can be computed for any parameter. The general method for estimating confidence intervals is presented in equation C-1.

$$CI = \text{parameter estimate} \pm (\text{critical value}) \times SE \qquad \text{Equation C-1}$$

The parameter estimate is the estimated value for the unknown population parameter. The critical value is the number, $z$, with probability, $p$, lying to its right (for an upper critical value) or left (for a lower critical value). For a standard normal distribution (i.e., arithmetic mean=0, standard

deviation=1), critical values are referred to as the *z-score* or *z-statistic*. These values are commonly given in statistics texts, and may also be calculated using the Microsoft Excel function *Normsinv(p)*, where *p* corresponds to the probability lying to the right of the value. Distributions that characterize parameter uncertainty are sometimes referred to as sampling distributions. The standard error (SE) is the standard deviation of the sampling distribution for the parameter estimate. The confidence interval conveys two concepts: (1) an upper and lower confidence limit (for a 2-sided CI), and (2) a confidence level ($1-\alpha$), which gives the probability that the method yields an interval that encloses the parameter (Moore and McCabe, 1993). Methods for estimating SE vary for specific parameters. For example, the SE of a mean concentration may be calculated based on the sample variance and the sample size (due to Central Limit Theorem). Methods for calculating the SE for other parameters, such as the 95$^{th}$ percentile, are more complex, and may be estimated from a series of nested bootstrap simulations (Efron and Tibshirani, 1993; U.S. EPA, 2001a).

When comparing alternative approaches for quantifying parameter uncertainty, criteria that are important to consider include the variance of the original data set, and the bias and coverage of the CIs generated by each method. In statistics, a method is unbiased if the mean of the sampling distribution is equal to the true value of the parameter. Similarly, a method has accurate coverage if the probability *p* that a CI does not cover the true parameter is equal to the probability level used to construct the CI. For risk assessment, the most desirable method is one that deals well with high variance, yields CIs that are sufficiently wide (i.e., the CI does not underestimate the probability of enclosing the population parameter), and, more specifically, yields upper confidence limits that are not biased low. The choice of the most appropriate method will depend on the characteristics of the data set and a balance between two objectives: (1) the desire to be health protective and, therefore, have a low probability of underestimating the mean, and (2) a desire to be accurate, in the sense of choosing a method whose expected coverage equals the true coverage. As a general principle for quantitative uncertainty analysis, if alternative methods yield very different answers, it is helpful to explore the reasons for the differences. The objective is to explain why the estimates of the 95% UCL differ, and to determine if the differences are sufficiently great that they could alter the risk management decision or PRG. This information should be presented as part of the risk communication process associated with the scientific management decision points of the tiered process for PRA (see Chapter 2).

As discussed in Chapter 5, in Superfund risk assessment, the EPC is usually calculated as the 95% UCL for the mean to account for the uncertainty in estimating the average concentration within an EU. The 95% UCL is defined as a value that, when repeatedly calculated for randomly drawn subsets of size (*n*), equals or exceeds the true population mean 95% of the time. In other words, it is calculated and applied as a 1-sided confidence limit. The 95% UCL is one percentile on the probability distribution that characterizes uncertainty in the mean (i.e., the PDFu for the mean). It is equal to the 95$^{th}$ percentile of the sampling distribution for the mean. EPA's guidance on calculating the concentration term describes the rationale and methodology for selecting the 95% UCL as the point estimate for the concentration term (U.S. EPA, 1992).

Common methodologies for characterizing the 95% UCL for the arithmetic mean concentration include the following: (1) application of Equation C-1 using Student's t-statistic (for normal distributions), (2) Land method using H-statistic (for lognormal distributions) (Land 1971, 1975), and (3) bootstrap and Jacknife resampling techniques (Efron and Tibshirani, 1993). Details on these methods and on choosing an appropriate method are provided in the ORD/OSWER guidance bulletin, *Lognormal Distribution in Environmental Applications* (U.S. EPA, 1997a), and the more recent OSWER guidance bulletin, *Guidance on Calculation of UCLs at Superfund Sites* (U.S. EPA, 2001a). An overview of

methods that may be used when data are not normal or lognormal is also provided by Schulz and Griffin (1999). It is the responsibility of the regional risk assessor to ensure that an appropriate method for calculating a UCL or for developing an uncertainty distribution is chosen. Chapter 3 (Table 3-1) provides an overview of approaches for characterizing uncertainty in the concentration term in both 1-D MCA and 2-D MCA.

### C.5.1 Quantifying Uncertainty without Information About Locations of Samples and Receptors

Knowledge of both the sampling locations and the receptor's activity patterns with the EU can be used to derive a more representative estimate of the 95% UCL. If a risk assessor has access to an environmental data set without information about the sample locations, the risk assessor is forced to assume that the sample consists of a number of independent observations. The validity of this assumption depends on the unknown spatial variability of contamination at the site. The size and location of an EU, as well as the choice of a statistical method for estimating the distribution of uncertainty around the mean concentration will require often implicit (and possibly incorrect) assumptions about the spatial distribution of contamination. Similarly, if information regarding receptor activity patterns is unavailable, one must assume that any area within the EU is equally representative of potential exposures. The risk assessor is urged to explore the effects of these various assumptions and to make choices that are protective of human health and the environment.

### C.5.2 Quantifying Uncertainty with Information About Locations of Samples and Receptors

In classical statistics, observations are assumed to be independent. This assumption is often invalid at contaminated sites where the method by which a chemical is released into the environment (e.g., deposition from airborne emissions; migration of contaminant plume from a point source) results in positive spatial autocorrelation. In other words, observations located next to each other tend to contain similar levels of contamination (i.e., redundant information) (Griffith and Layne, 1999). For example, the higher the spatial autocorrelation, the less incremental information is provided by adding observations in close proximity to existing observations. This decrease in the information content of a site sample is exacerbated by the tendency to choose sampling locations in the most contaminated areas rather than distributed at regular spatial intervals or specified using random sampling methodology.

At many hazardous waste sites, environmental sampling plans are designed with remedial actions rather than risk assessment in mind. Therefore, the risk assessor must establish a correspondence between the actual sampling locations and the locations a receptor would be expected to frequent. Geostatistics may provide information to establish this correspondence.

Geostatistics is a branch of spatial statistics that can be used to model spatial variability and parameter uncertainty. Geostatistics offers two fundamental contributions to risk assessment: (1) a group of methods to describe the spatial distribution of a contaminant in a quantitative fashion, and (2) the ability to maximize the information available in the data set (Deutsch and Journel, 1988; Isaacs and Srivastava, 1989).

Geostatistics is capable of using the information revealed by a correlation analysis of the data to estimate concentrations at unsampled locations. For example, geostatistics is able to use the spatial information contained in the data to model uncertainty in contaminant concentrations for areas where

data are sparse, a situation commonly encountered in site assessment work. Using geostatistics, information from samples collected from outside an EU can be used to model the uncertainty in the mean concentration within an EU. Approaches that do not consider the geospatial information present in the data are limited to the subset of samples within an EU. However, this ability to model uncertainty in areas where data are sparse is also limited, and a well characterized site is still the best path to understanding the risk at that site.

Geostatistical methods may be used to calculate a distribution of uncertainty in the mean of the concentration term for use in PRAs. In the past, geostatistics has not been widely applied to risk assessment, even though uncertainty in the exposure concentration is often a major source of uncertainty in risk estimates. Most risk assessors quantify uncertainty in the long-term average concentration without explicitly considering the spatial information present in data obtained from environmental sampling or knowledge of the receptor's movement and activities within the EU. When spatial information does not exist, the inherent assumption is that environmental sampling yields a data set that is representative of the spatial variability in concentrations encountered by a receptor. This assumption represents one source of uncertainty in the EPC. In addition, data collected outside an EU are often ignored in the analysis, even though they can provide a more comprehensive view of patterns of contamination across the site, including the EU of interest. Ignoring site-wide information may result in less informed estimates of risk and, therefore, less effective remedial designs (i.e., too little or too much remediation). In the past five years, with rapidly expanding software and hardware capabilities, some examples of the application of geostatistics can be found in exposure assessment and remedial design (e.g., Gomez-Hernandez, 1996; Goovaerts, 1996, 1997; Kriakidis, 1996; Ginevan and Splitstone, 1997; McKenna, 1997, 1998) as well as site assessment guidance (e.g., U.S. EPA, 2000).

A limit to applying geostatistics at hazardous waste sites is that the method is resource intensive and requires personnel experienced with the software and techniques. Risk assessors and risk managers should ensure that contractors and other personnel have the necessary capabilities before applying geostatistical methods to risk assessment or site cleanup. Geostatistics is a powerful tool, but it cannot incorporate quantitative knowledge regarding all sources of uncertainty. The risk assessor is cautioned to consider all possible sources of uncertainty as described in Chapter 5. As indicated previously, a full discussion of geostatistics is beyond the scope of this guidance, and interested readers are urged to consult the OSWER guidance document, *Guidance on Strategy for Surface Soil Cleanup at Superfund Sites* (U.S. EPA, 2001b).

EPA has produced several software packages used for geostatistical estimation. Among these are GEO-EAS and GEO-PACK. Expertise in geostatistics can be obtained from ORD/Las Vegas.

## REFERENCES FOR APPENDIX C

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